

## Author index to volume 282

- Abe, K., see Takahashi, K. 282 (1998) 361  
Achiba, Y., see Kohno, M. 282 (1998) 330  
Aflatooni, K., G.A. Gallup and P.D. Burrow, Dissociative electron attachment in chloroalkanes and the correlation with vertical attachment energies 282 (1998) 398  
Aguilar, A., see Huarte-Larrañaga, F. 282 (1998) 91  
Aicher, K.P., C. Weickhardt and J. Grotemeyer, Simultaneous determination of absorption cross sections and decay rate constants by quantitative laser mass spectrometry 282 (1998) 257  
Albertí, M., see Huarte-Larrañaga, F. 282 (1998) 91  
Alvariño, J.M., see Huarte-Larrañaga, F. 282 (1998) 91  
Alves Jr., S., see Malta, O.L. 282 (1998) 233  
An, X., F. Jiang, C. Chen and W. Shen, Molar mass dependence of critical amplitudes for chain-molecule solutions 282 (1998) 403  
Ananchenko, G.S., E.G. Bagryanskaya and R.Z. Sagdeev, Low magnetic field electron–nuclear resonance transitions detected by nuclear polarization of radical reaction products 282 (1998) 450  
Arnold, D.W., M. Korolik, C. Wittig and H. Reisler, The effect of translational energy on collision-induced dissociation of highly excited NO<sub>2</sub> on MgO(100) 282 (1998) 313  
Arthur, N.L. and L.A. Miles, Rate constants for H + (CH<sub>3</sub>)<sub>4–n</sub>SiH<sub>n</sub>, n = 1–4 282 (1998) 192  
Ayappa, K.G., Influence of temperature on mixture adsorption in carbon nanotubes: a grand canonical Monte Carlo study 282 (1998) 59  
  
Bagryanskaya, E.G., see Ananchenko, G.S. 282 (1998) 450  
Bai, J., see Wang, L. 282 (1998) 204  
Baran, E.J., see Sáez-Puche, R. 282 (1998) 273  
Belosludov, V.R., see Shpakov, V.P. 282 (1998) 107  
Benter, Th., see Schmidt, S. 282 (1998) 292  
Bousseksou, A., L. Salmon, F. Varret and J.-P. Tuchagues, The second example of spin conversion governed by molecular vibrations: a novel ferrous complex resulting from hexacoordination of a Schiff base with an N<sub>4</sub>O<sub>2</sub> donor set 282 (1998) 209  
Brito, H.F., see Malta, O.L. 282 (1998) 233  
Buijsse, B., see Shiau, T.P. 282 (1998) 369  
Bunker, P.R., see East, A.L.L. 282 (1998) 49  
Burrow, P.D., see Aflatooni, K. 282 (1998) 398  
Bytheway, I. and M.W. Wong, The prediction of vibrational frequencies of inorganic molecules using density functional theory 282 (1998) 219  
  
Cai, Z.-L. and J.P. François, An internally contracted multireference configuration interaction analysis of the SiO<sup>+</sup> B<sup>2</sup>Σ<sup>+</sup>–X<sup>2</sup>Σ<sup>+</sup> transition moment 282 (1998) 29

- Changenet, P., H. Zhang, M.J. van der Meer, K.J. Hellingwerf and M. Glasbeek, Subpicosecond fluorescence upconversion measurements of primary events in yellow proteins 282 (1998) 276
- Chen, C., see An, X. 282 (1998) 403
- Choi, C.H. and M. Kertesz, Is a 1.90 Å C–C bond length in polymeric fullerenes possible? 282 (1998) 318
- Christiansen, O., see Hättig, C. 282 (1998) 139
- Chu, S.-Y., see Su, M.-D. 282 (1998) 25
- Clementi, E. and G. Corongiu, Molecular correlation energy with the HF–CC method 282 (1998) 335
- Compton, R.N., see Ying, Z.C. 282 (1998) 268
- Copeland, R.A., see Shiau, T.P. 282 (1998) 369
- Corongiu, G., see Clementi, E. 282 (1998) 335
- Das, S.K., see Mukherjee, T. 282 (1998) 64
- Daum, R., see Tietz, C. 282 (1998) 164
- De Backer, S., see Scheblykin, I.G. 282 (1998) 250
- De Mello Donegá, C., see Malta, O.L. 282 (1998) 233
- Dennis, C.R., C.J. Whitham, R.J. Low and B.J. Howard, Novel magnetic interactions in the open-shell NO–HF complex 282 (1998) 421
- Diraison, M., P. Millie, S. Pommeret, T. Gustavsson and J.-Cl. Mialocq, Solvation structure of coumarin 1 in acetonitrile: role of the electrostatic solute–solvent potential 282 (1998) 152
- Dräbenstedt, A., see Tietz, C. 282 (1998) 164
- Dutta-Roy, B., see Mukherjee, T. 282 (1998) 64
- East, A.L.L. and P.R. Bunker, An ab initio calculation of the rotation and internal-rotation energy levels of the ethyl radical 282 (1998) 49
- Ehara, M. and H. Nakatsuji, Outer- and inner-valence ionization spectra of N<sub>2</sub> and CO: SAC-CI(general-R) compared with full-CI spectra 282 (1998) 347
- Esenaliev, R.O., see Shelimov, K.B. 282 (1998) 429
- Faigel, G., see Pekker, S. 282 (1998) 435
- Feng, J., see Ge, M. 282 (1998) 54
- Fiebig, T., W. Kühnle and H. Staerk, Electronic interaction and charge transfer efficiencies in triaromatic donor–acceptor systems. An experimental and theoretical study 282 (1998) 7
- Fleury, L., see Tietz, C. 282 (1998) 164
- François, J.P., see Cai, Z.-L. 282 (1998) 29
- Fujisawa, J., Y. Ohba and S. Yamauchi, Direct observation of electron spin polarization transfer in triplet–triplet energy transfer between porphyrins and fullerene in fluid solution 282 (1998) 181
- Fukazawa, H., S. Ikeda and S. Mae, Incoherent inelastic neutron scattering measurements on ice XI; the proton-ordered phase of ice I<sub>h</sub> doped with KOH 282 (1998) 215
- Furlan, A., H.A. Scheld and J.R. Huber, Production of OCCN radicals by photodissociation of carbonyl cyanide CO(CN)<sub>2</sub> at 193 nm 282 (1998) 1
- Gabuda, S.P., S.G. Kozlova, O.B. Lapina and V.V. Terskikh, <sup>125</sup>Te NMR in TeO<sub>2</sub> single crystal: Te–Te chemical bonding and tunneling of 5s<sup>2</sup> electrons 282 (1998) 245
- Gallup, G.A., see Aflatoon, K. 282 (1998) 398
- Ge, M., J. Feng, W. Tian, Z. Li, X. Huang and C. Sun, Ab initio SCF calculations of Ti<sub>8</sub>C<sub>12</sub>(H<sub>2</sub>O)<sub>8</sub> and Ti<sub>8</sub>C<sub>12</sub>(C<sub>2</sub>H<sub>4</sub>)<sub>4</sub>. An investigation on reactions of titanium–carbon cluster 282 (1998) 54
- Giménez, X., see Huarte-Larrañaga, F. 282 (1998) 91

- Glasbeek, M., see Changenet, P. 282 (1998) 276  
Gonçalves e Silva, F.R., see Malta, O.L. 282 (1998) 233  
González-Baró, A.C., see Sáez-Puche, R. 282 (1998) 273  
Görner, H., Photochemical ring opening in nitrospiropyrans: triplet pathway and the role of singlet molecular oxygen 282 (1998) 381  
Görner, H., see Sadvovskii, N.A. 282 (1998) 456  
Grage, M.M.-L., T. Keszthelyi, J.F. Offersgaard and R. Wilbrandt, Bithiophene radical cation: resonance Raman spectroscopy and molecular orbital calculations 282 (1998) 171  
Gregory, J.K., The dipole moment of the water dimer 282 (1998) 147  
Grotemeyer, J., see Aicher, K.P. 282 (1998) 257  
Gruber, A., see Tietz, C. 282 (1998) 164  
Gustavsson, T., see Diraison, M. 282 (1998) 152  
  
Haglund Jr., R.F., see Ying, Z.C. 282 (1998) 268  
Halberstadt, N. and K.C. Janda, The resonant charge hopping rate in positively charged helium clusters 282 (1998) 409  
Han, J., Energetics and structures of fullerene crop circles 282 (1998) 187  
Hättig, C., O. Christiansen and P. Jørgensen, Frequency-dependent second hyperpolarizabilities using coupled cluster cubic response theory 282 (1998) 139  
Havenith, R.W.A., L.W. Jenneskens and J.H. van Lenthe, The effect of syn-anti isomerism on the lowest valence transitions of 1,1'-bicyclohexylidene. An ab initio MRDCI investigation 282 (1998) 39  
Hellingwerf, K.J., see Changenet, P. 282 (1998) 276  
Hishikawa, A., A. Iwamae, K. Hoshina, M. Kono and K. Yamanouchi, Mass-resolved two-dimensional momentum imaging of the Coulomb explosion of N<sub>2</sub> and SO<sub>2</sub> in an intense laser field 282 (1998) 283  
Hoshina, K., see Hishikawa, A. 282 (1998) 283  
Howard, B.J., see Dennis, C.R. 282 (1998) 421  
Huang, X., see Ge, M. 282 (1998) 54  
Huarte-Larrañaga, F., X. Giménez, M. Albertí, A. Aguilar, A. Laganà and J.M. Alvarino, Energy mode effectiveness and tunnelling in triatomic reactions: the energy threshold for the Mg + FH → MgF + H reaction 282 (1998) 91  
Huber, J.R., see Furlan, A. 282 (1998) 1  
Huffman, C.B., see Shelimov, K.B. 282 (1998) 429  
Hwang, E.S., see Shiau, T.P. 282 (1998) 369  
  
Ibuki, T., see Uchida, S. 282 (1998) 375  
Ikeda, S., see Fukazawa, H. 282 (1998) 215  
Ikeguchi, M., see Shimizu, S. 282 (1998) 79  
Inoue, T., see Kawazumi, H. 282 (1998) 159  
Ishida, H., Y. Nagai and A. Kidera, Symplectic integrator for molecular dynamics of a protein in water 282 (1998) 115  
Ishii, C., see Kaneko, K. 282 (1998) 176  
Iwamae, A., see Hishikawa, A. 282 (1998) 283  
  
Janda, K.C., see Halberstadt, N. 282 (1998) 409  
Jenneskens, L.W., see Havenith, R.W.A. 282 (1998) 39  
Jiang, F., see An, X. 282 (1998) 403



- Jonah, C.D., see Takahashi, K. 282 (1998) 361
- Jørgensen, P., see Hättig, C. 282 (1998) 139
- Kaieda, T., see Kawazumi, H. 282 (1998) 159
- Kaneko, K., J. Suzuki and C. Ishii, Low temperature magnetic properties of an O<sub>2</sub> and H<sub>2</sub>O mixed molecular assembly, confined in a graphitic nanospace 282 (1998) 176
- Kawazumi, H., T. Kaieda, T. Inoue and T. Ogawa, Development of an interfacial thermal lens technique: monitoring the dissolving process of amphiphilic molecules at the hexane-water interface 282 (1998) 159
- Kertesz, M., see Choi, C.H. 282 (1998) 318
- Keszthelyi, T., see Grage, M.M.-L. 282 (1998) 171
- Kidera, A., see Ishida, H. 282 (1998) 115
- Kobayashi, K. and S. Nagase, Structures and electronic states of M@C<sub>82</sub> (M = Sc, Y, La and lanthanides) 282 (1998) 325
- Kohno, M., S. Suzuki, H. Shiromaru, T. Moriwaki and Y. Achiba, Ultraviolet photoelectron spectroscopy on the linear conformer of negatively charged carbon clusters C<sub>n</sub><sup>-</sup> (10 ≤ n ≤ 16) 282 (1998) 330
- Kono, M., see Hishikawa, A. 282 (1998) 283
- Kono, M., see Uchida, S. 282 (1998) 375
- Koper, M.T.M. and G.A. Voth, A theory for adiabatic bond breaking electron transfer reactions at metal electrodes 282 (1998) 100
- Korolik, M., see Arnold, D.W. 282 (1998) 313
- Kozlova, S.G., see Gabuda, S.P. 282 (1998) 245
- Kühnle, W., see Fiebig, T. 282 (1998) 7
- Kuzmin, M.G., see Sadovskii, N.A. 282 (1998) 456
- Kvamme, B., see Shpakov, V.P. 282 (1998) 107
- Laganà, A., see Huarte-Larrañaga, F. 282 (1998) 91
- Lahamer, A.S., see Ying, Z.C. 282 (1998) 268
- Lapina, O.B., see Gabuda, S.P. 282 (1998) 245
- Lewis, J.E. and M. Maroncelli, On the (uninteresting) dependence of the absorption and emission transition moments of coumarin 153 on solvent 282 (1998) 197
- Li, H., see Wang, L. 282 (1998) 204
- Li, Z., see Ge, M. 282 (1998) 54
- Lopinski, G.P., D.J. Moffatt and R.A. Wolkow, Benzene/Si(100): metastable chemisorption and binding state conversion 282 (1998) 305
- Low, R.J., see Dennis, C.R. 282 (1998) 421
- Lu, R., see Wang, L. 282 (1998) 204
- Mae, S., see Fukazawa, H. 282 (1998) 215
- Malcolm, N.O.J. and J.J.W. McDouall, A simple scaling for combining multiconfigurational wavefunctions with density functionals 282 (1998) 121
- Malta, O.L., H.F. Brito, J.F.S. Menezes, F.R. Gonçalves e Silva, C. de Mello Donegá and S. Alves Jr., Experimental and theoretical emission quantum yield in the compound Eu(thenoyltrifluoroacetate)<sub>3</sub>.2(dibenzyl sulfoxide) 282 (1998) 233
- Manthe, U. and F. Matzkies, Quantum calculations of thermal rate constants and reaction probabilities: H<sub>2</sub> + CN → H + HCN 282 (1998) 442
- Maroncelli, M., see Lewis, J.E. 282 (1998) 197

- Martin, J.M.L. and O. Uzan, Basis set convergence in second-row compounds. The importance of core polarization functions 282 (1998) 16
- Matzkies, F., see Manthe, U. 282 (1998) 442
- McDouall, J.J.W., see Malcolm, N.O.J. 282 (1998) 121
- Menezes, J.F.S., see Malta, O.L. 282 (1998) 233
- Mhaka, A.M. and P.E. Siska, Dynamics of molecular Penning ionization: angle-energy distributions of  $N_2^+$  from  $He^*(2^1S) + N_2$  282 (1998) 299
- Mialocq, J.-Cl., see Diraison, M. 282 (1998) 152
- Miles, L.A., see Arthur, N.L. 282 (1998) 192
- Millie, P., see Diraison, M. 282 (1998) 152
- Mitra, S. and N. Tamai, Femtosecond spectroscopic study on photochromic salicylideneaniline 282 (1998) 391
- Moffatt, D.J., see Lopinski, G.P. 282 (1998) 305
- Moriwaki, T., see Kohno, M. 282 (1998) 330
- Mosyak, A., P.J. Rossky and L. Turi, A dynamical analysis of energy level fluctuations for an excess electron in methanol 282 (1998) 239
- Mukherjee, T., S.K. Das, B. Nandi Ganguly, P. Sen and B. Dutta-Roy, Positronium formation in a reverse micellar system 282 (1998) 64
- Nagai, Y., see Ishida, H. 282 (1998) 115
- Nagase, S., see Kobayashi, K. 282 (1998) 325
- Nakamura, A., see Takahashi, H. 282 (1998) 128
- Nakatsuji, H., see Ehara, M. 282 (1998) 347
- Nandi Ganguly, B., see Mukherjee, T. 282 (1998) 64
- Nitta, T., see Takahashi, H. 282 (1998) 128
- Offersgaard, J.F., see Grage, M.M.-L. 282 (1998) 171
- Ogawa, T., see Kawazumi, H. 282 (1998) 159
- Ohba, Y., see Fujisawa, J. 282 (1998) 181
- Oszlányi, G., see Pekker, S. 282 (1998) 435
- Pekker, S., G. Oszlányi and G. Faigel, Structure and stability of covalently bonded polyfulleride ions in  $A_xC_{60}$  salts 282 (1998) 435
- Pérez-Jordá, J.M. and W. Yang, On the scaling of multipole methods for particle-particle interactions 282 (1998) 71
- Pommeret, S., see Diraison, M. 282 (1998) 152
- Reisler, H., see Arnold, D.W. 282 (1998) 313
- Remko, M. and M. Šarišský, Structure and gas phase stability of complexes  $L...M$ , where  $M = Li^+, Na^+$  and  $Mg^{2+}$ , and  $L = H_2O, H_2S, SiH_2, NH_3$  and their methyl derivatives 282 (1998) 227
- Rinzler, A.G., see Shelimov, K.B. 282 (1998) 429
- Robie, D.C., see Seiser, N. 282 (1998) 263
- Romero, J., see Sáez-Puche, R. 282 (1998) 273
- Rosky, P.J., see Mosyak, A. 282 (1998) 239
- Sadovskii, N.A., M.G. Kuzmin, H. Görner and K. Schaffner, Temperature effects on radical ion and triplet quantum yields in excited-state electron transfer reactions of 1,12-benzperylene in acetonitrile 282 (1998) 456
- Sáez-Puche, R., J. Romero, A.C. González-Baró and E.J. Baran, Magnetic behaviour of bis(5,7-dichloro-8-hydroxyquinolinato)oxovanadium(IV)

- Sagdeev, R.Z., see Ananchenko, G.S. 282 (1998) 273
- Saito, K., see Uchida, S. 282 (1998) 450
- Salmon, L., see Bousseksou, A. 282 (1998) 375
- Šarišský, M., see Remko, M. 282 (1998) 209
- Sawamura, S., see Takahashi, K. 282 (1998) 227
- Schaffner, K., see Sadovskii, N.A. 282 (1998) 361
- Scheblykin, I.G., O.P. Varnavsky, W. Verbouwe, S. De Backer, M. Van der Auweraer and A.G. Vitukhnovsky, Relaxation dynamics of excitons in J-aggregates revealing a two-component Davydov splitting 282 (1998) 456
- Scheld, H.A., see Furlan, A. 282 (1998) 250
- Schindler, R.N., see Schmidt, S. 282 (1998) 1
- Schmidt, S., Th. Benter and R.N. Schindler, Photodissociation dynamics of ClO radicals in the range ( $237 \leq \lambda \leq 270$ ) nm and at 205 nm and the velocity distribution of O(<sup>1</sup>D) atoms 282 (1998) 292
- Schuster, J., see Tietz, C. 282 (1998) 164
- Seiser, N. and D.C. Robie, Pressure broadening in the oxygen  $b^1\Sigma_g^+(v' = 1) \leftarrow X^3\Sigma_g^-(v'' = 0)$  band measured by cavity ring-down spectroscopy 282 (1998) 263
- Sen, P., see Mukherjee, T. 282 (1998) 64
- Shelimov, K.B., R.O. Esenaliev, A.G. Rinzler, C.B. Huffman and R.E. Smalley, Purification of single-wall carbon nanotubes by ultrasonically assisted filtration 282 (1998) 429
- Shen, W., see An, X. 282 (1998) 403
- Shiau, T.P., E.S. Hwang, B. Buijsse and R.A. Copeland, Vibrational-level-dependent yields of O<sub>2</sub>( $b^1\Sigma_g^+$ ,  $v = 0$ ) following collisional removal of O<sub>2</sub>( $A^3\Sigma_u^+$ ,  $v$ ) 282 (1998) 369
- Shimizu, K., see Shimizu, S. 282 (1998) 79
- Shimizu, S., M. Ikeguchi and K. Shimizu, An off-lattice theory of solvation: extension of the Flory  $\chi$  parameter into continuum space 282 (1998) 79
- Shiromaru, H., see Kohno, M. 282 (1998) 330
- Shpakov, V.P., J.S. Tse, C.A. Tulk, B. Kvamme and V.R. Belosludov, Elastic moduli calculation and instability in structure I methane clathrate hydrate 282 (1998) 107
- Shushin, A.I., Manifestation of spin exchange relaxation in microwave field induced magnetic field effects on recombination of confined radical pairs 282 (1998) 413
- Siska, P.E., see Mhaka, A.M. 282 (1998) 299
- Sjövall, P. and P. Uvdal, Oxygen sticking on Pd(111): double precursors, corrugation and substrate temperature effects 282 (1998) 355
- Smalley, R.E., see Shelimov, K.B. 282 (1998) 429
- Staerk, H., see Fiebig, T. 282 (1998) 7
- Su, M.-D. and S.-Y. Chu, Theoretical model for oxidative activation of the O-H bond to platinum(0) complexes 282 (1998) 25
- Sun, C., see Ge, M. 282 (1998) 54
- Suzuki, J., see Kaneko, K. 282 (1998) 176
- Suzuki, S., see Kohno, M. 282 (1998) 330
- Tabayashi, K., see Uchida, S. 282 (1998) 375
- Takahashi, H., A. Nakamura and T. Nitta, Effect of the shape of simulation box on the Van der Waals loop of a Lennard-Jones fluid 282 (1998) 128
- Takahashi, K., K. Abe, S. Sawamura and C.D. Jonah, Spectroscopic study of 4-aminobenzophenone in supercritical CF<sub>3</sub>H and CO<sub>2</sub>: local density and Onsager's reaction cavity radius 282 (1998) 361



- Takahashi, O., see Uchida, S. 282 (1998) 375  
Tamai, N., see Mitra, S. 282 (1998) 391  
Tanaka, H., Cavity distribution in liquid water and hydrophobic hydration 282 (1998) 133  
Tanaka, M., see Uchida, S. 282 (1998) 375  
Terskikh, V.V., see Gabuda, S.P. 282 (1998) 245  
Tian, W., see Ge, M. 282 (1998) 54  
Tietz, C., R. Daum, A. Dräbenstedt, J. Schuster, L. Fleury, A. Gruber, J. Wrachtrup and C. von Borczyskowski, Correlation spectroscopy of individual molecules immobilized on surfaces under ambient conditions 282 (1998) 164  
Tse, J.S., see Shpakov, V.P. 282 (1998) 107  
Tuchagues, J.-P., see Bousseksou, A. 282 (1998) 209  
Tulk, C.A., see Shpakov, V.P. 282 (1998) 107  
Turi, L., see Mosyak, A. 282 (1998) 239  
  
Uchida, S., K. Tabayashi, M. Tanaka, O. Takahashi, K. Saito, M. Kono and T. Ibuki, Photoabsorption and fluorescence excitation of malononitrile in the vacuum UV region 282 (1998) 375  
Uvdal, P., see Sjövall, P. 282 (1998) 355  
Uzan, O., see Martin, J.M.L. 282 (1998) 16  
  
Van der Auweraer, M., see Scheblykin, I.G. 282 (1998) 250  
Van der Meer, M.J., see Changenet, P. 282 (1998) 276  
Van Lenthe, J.H., see Havenith, R.W.A. 282 (1998) 39  
Varnavsky, O.P., see Scheblykin, I.G. 282 (1998) 250  
Varret, F., see Bousseksou, A. 282 (1998) 209  
Verbouwe, W., see Scheblykin, I.G. 282 (1998) 250  
Vitukhnovsky, A.G., see Scheblykin, I.G. 282 (1998) 250  
Von Borczyskowski, C., see Tietz, C. 282 (1998) 164  
Voth, G.A., see Koper, M.T.M. 282 (1998) 100  
  
Wang, L., H. Li, J. Bai and R. Lu, A novel method for the generation of high Rydberg states of atoms and molecules 282 (1998) 204  
Weickhardt, C., see Aicher, K.P. 282 (1998) 257  
Whitham, C.J., see Dennis, C.R. 282 (1998) 421  
Wilbrandt, R., see Grage, M.M.-L. 282 (1998) 171  
Wittig, C., see Arnold, D.W. 282 (1998) 313  
Wolkow, R.A., see Lopinski, G.P. 282 (1998) 305  
Wong, M.W., see Bytheway, I. 282 (1998) 219  
Wrachtrup, J., see Tietz, C. 282 (1998) 164  
  
Yamanouchi, K., see Hishikawa, A. 282 (1998) 283  
Yamauchi, S., see Fujisawa, J. 282 (1998) 181  
Yang, W., see Pérez-Jordá, J.M. 282 (1998) 71  
Yavas, O., see Ying, Z.C. 282 (1998) 268  
Ying, Z.C., A.S. Lahamer, O. Yavas, R.F. Haglund Jr. and R.N. Compton, Infrared absorption spectroscopy using a free-electron laser 282 (1998) 268  
  
Zhang, H., see Changenet, P. 282 (1998) 276